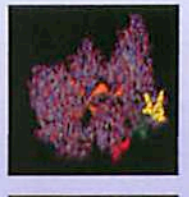
X-Rays, Lasers, and Molecular Movies

or

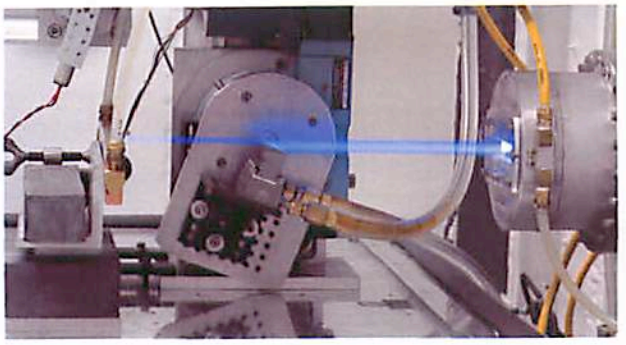
Fiat Lux: what's under the dome up the hill?

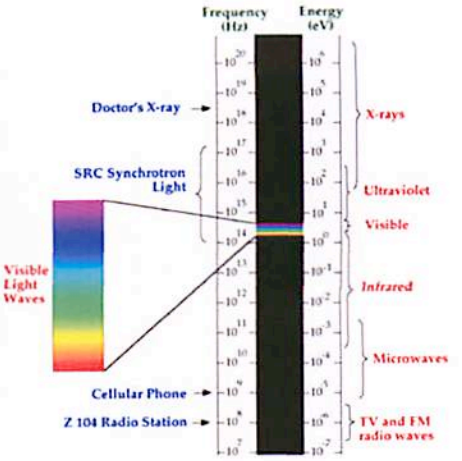
Roger Falcone

Physics Department, UC Berkeley
Advanced Light Source, LBNL

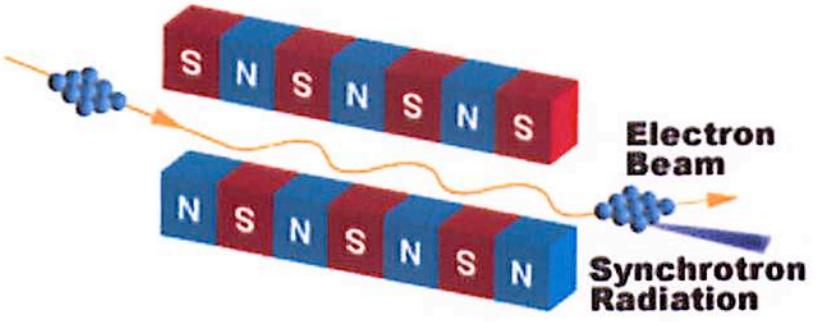


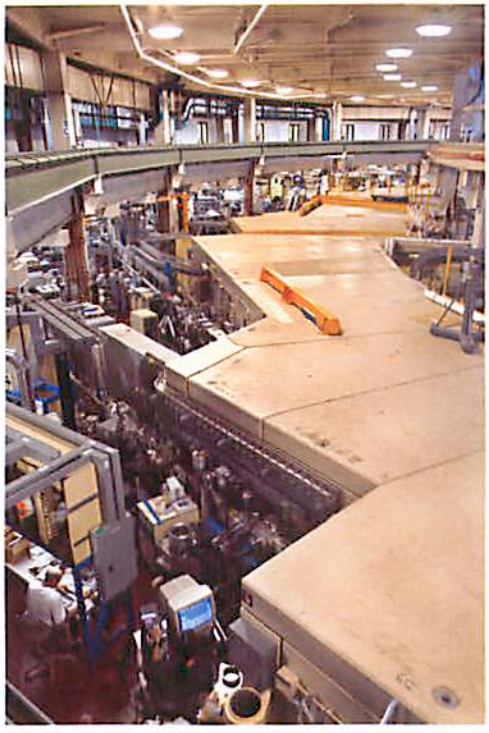
Nano*High December 13, 2008

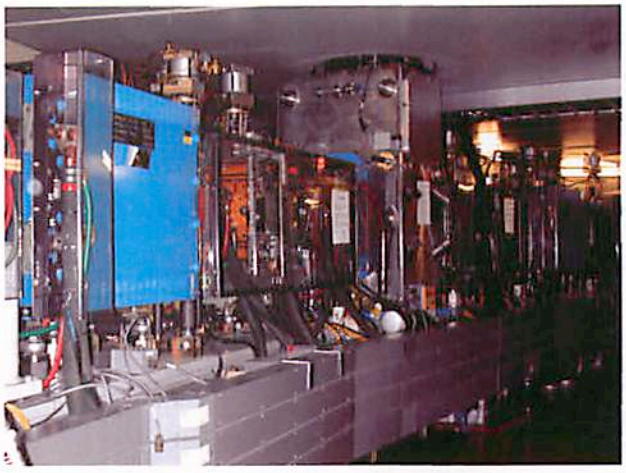




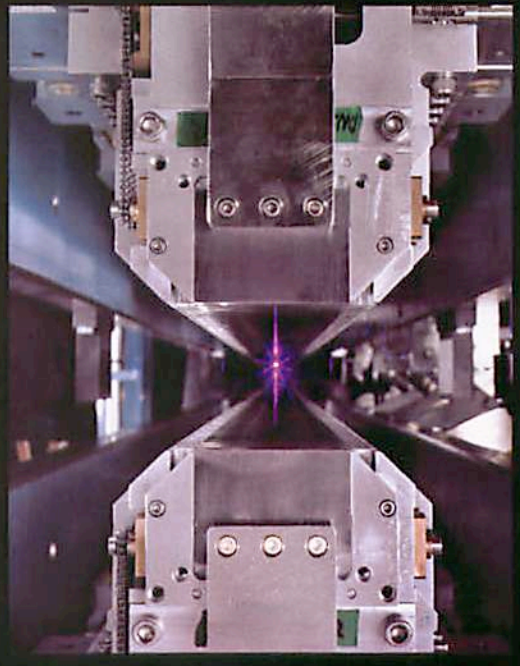
"synchrotron" x-ray pulses
are produced by relativistic electron bunches in accelerators
when the electrons pass through periodic magnetic fields



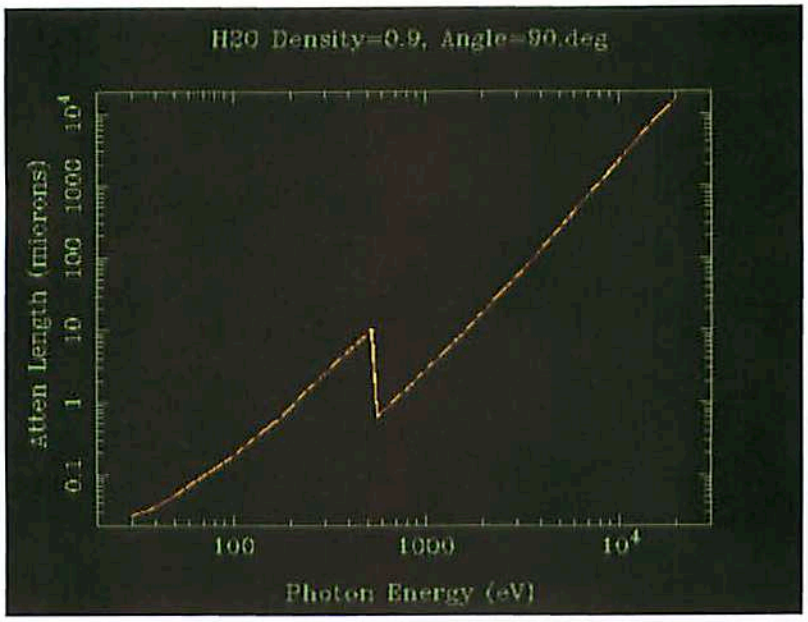




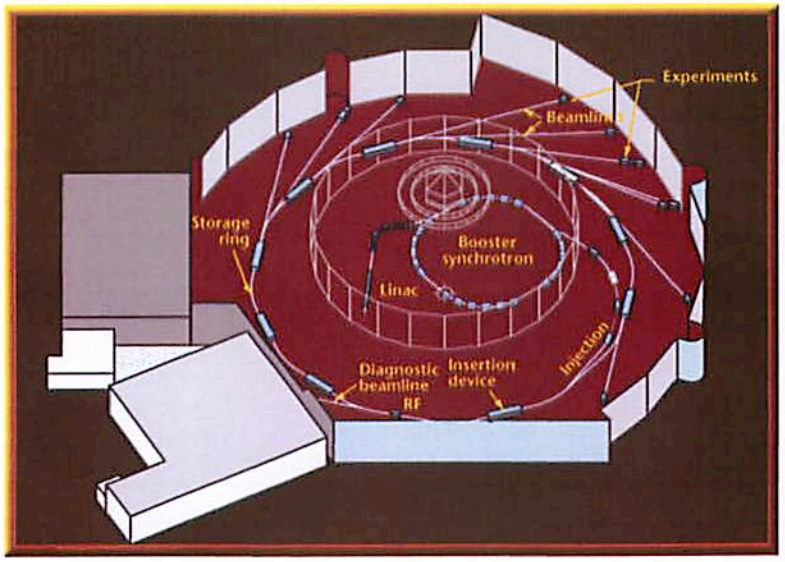
Undulator / Wiggler



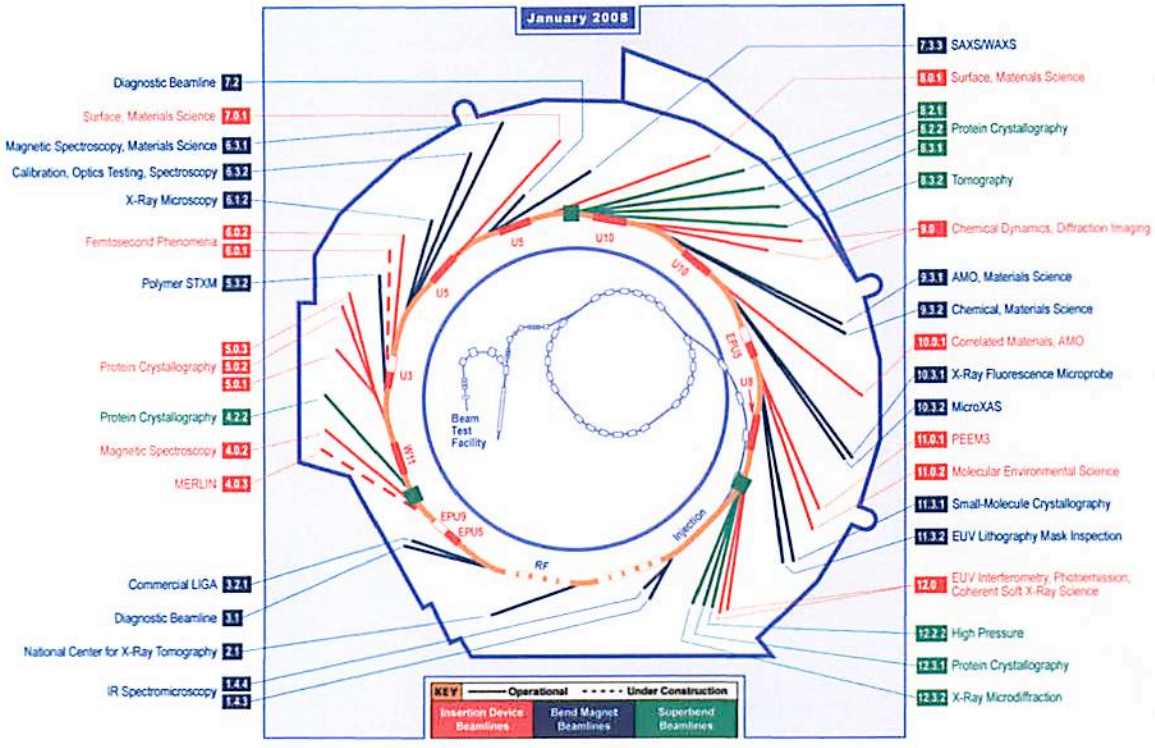
absorption of x-rays



Storage ring x-ray sources



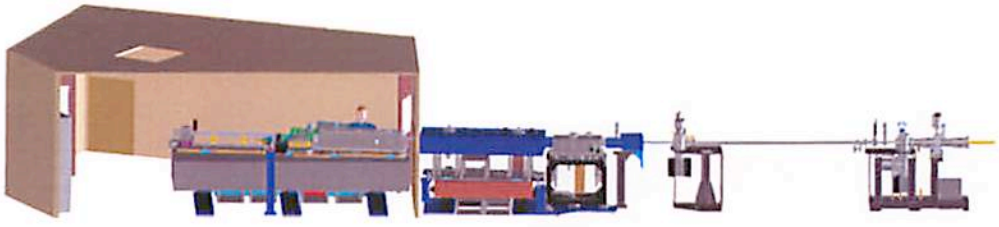
Beamlines at the ALS 2008



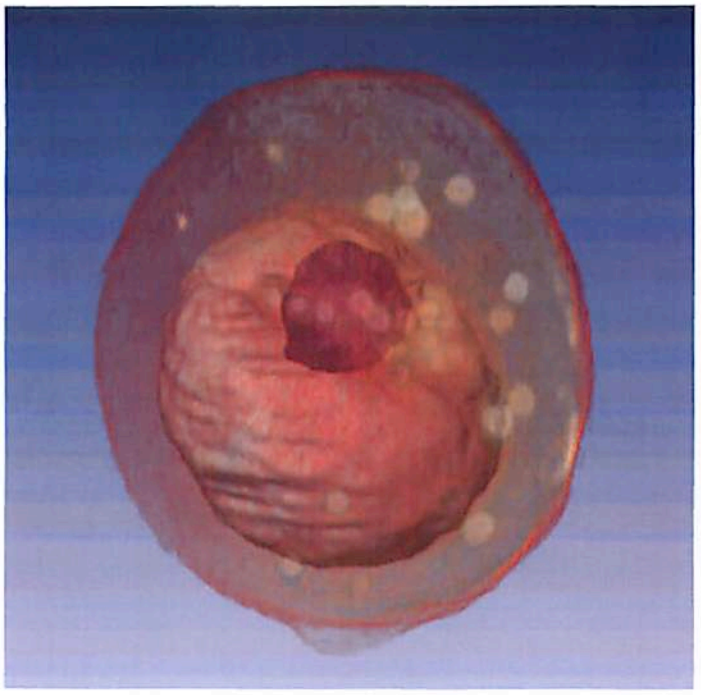
Biomedical imaging at the ALS

The National Center for X-Ray Tomography

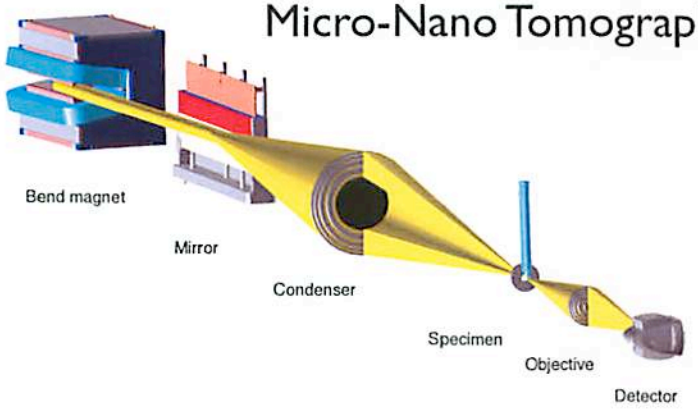
Director: Carolyn Larabell (UCSF/LBNL)

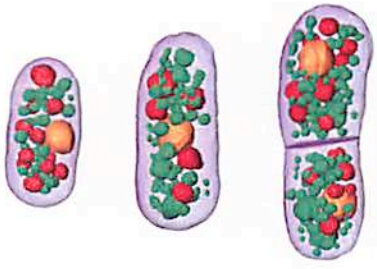


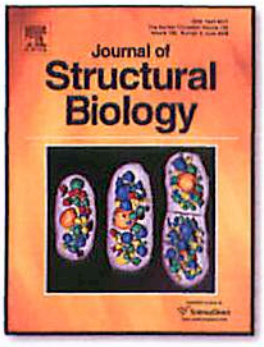
3-d x-ray tomography of a cell



Micro-Nano Tomography / Radiography







Segmented using organelle appearance:

Mitochondria

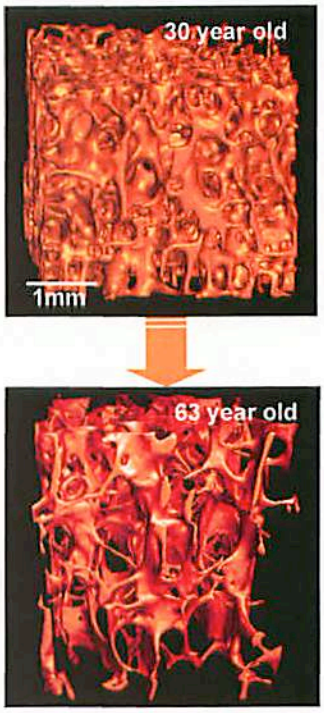
Other organelles

D.Y. Parkinson, G. McDermott, L.D. Etkin, M.A. Le Gros & C.A. Larabell (2008) J. Structural Biology 162:380-386.

Micro X-ray Tomography of Trabecular bone decay in vertebrae

Photon energy 10-40KeV
Full field imaging with scintillator and visible light magnification optics.
Resolution 3um

The internal structure of vertebra is Trabecular bone (spongy bone) – carries 90% of the force Osteoporis is the weakening and collapse of this structure.

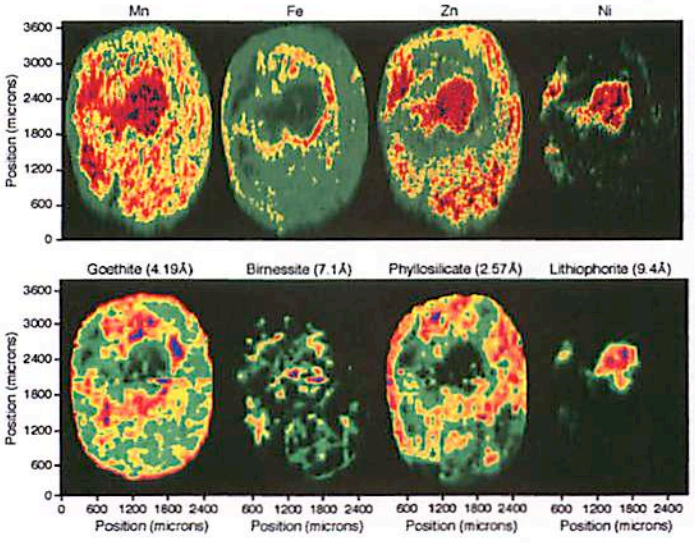


J.Kinney et al.Bone, **36**, 193-201 (2005)

Osteoporosis studies

Osteoporosis is not entirely explained by loss of bone mass. Some people loose bone mass and do not gets fractures – others are the opposite.

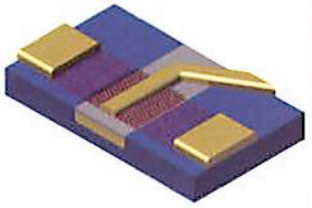
TRACE METALS IN SOILS AND SEDIMENTS



Three X-Ray Micro Techniques Focus on Nickel and Zinc Sequestration

A. Manceau (Université Joseph Fourier and CNRS, France, and ALS); N. Tamura, M.A. Marcus, A.A. MacDowell, R.S. Celestre, R.E. Sublett, and H.A. Padmore (ALS); and G. Sposito (Berkeley Lab). [*American Mineralogist* **87**, 1494 (2002)]

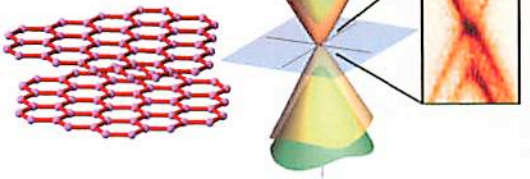
Graphene: a new material for high performance electronics



- Graphene, a single layer of carbon, is the building block of graphite, nanotubes, buckyballs.
- A bilayer of graphene can be a switch <1 nm thick for high current densities (~10^8 A/cm^2).

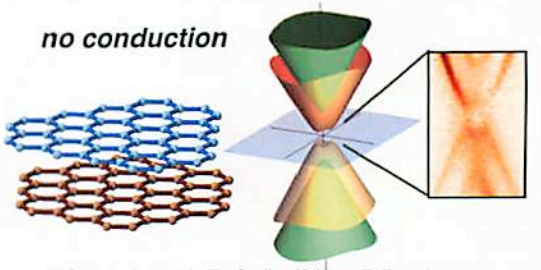
Unbiased

conduction



Biased

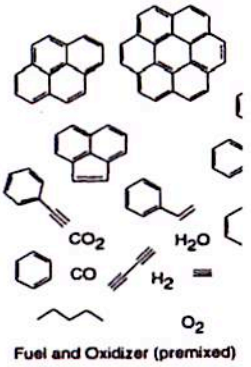
no conduction



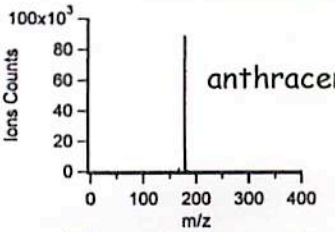
T. Ohta, A. Bostwick, Th. Seyller, K. Horn, E. Rotenberg, Science, 2006. 313: p. 951-954.

Combustion Chemistry

Sandia National Lab, ALS

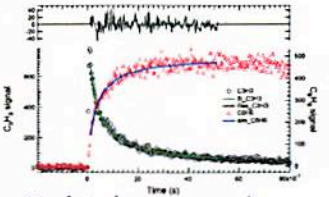


Fuel and Oxidizer (premixed)

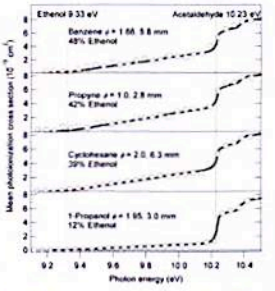


Fragment free mass spectrometry

$C_3H_3 + C_3H_3 \rightarrow C_6H_6$

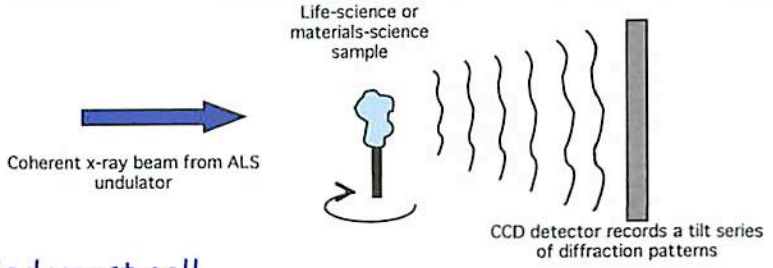


Multiplexing and universal detection

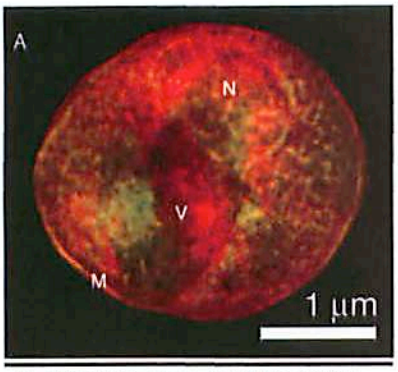


Enol formation in flames
Isomer selectivity

Diffraction Microscopy

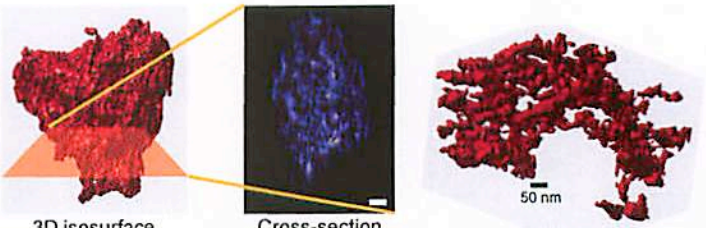


Freeze dried yeast cell



D. Shapiro et al, PNAS 2005

Tantalum oxide foam

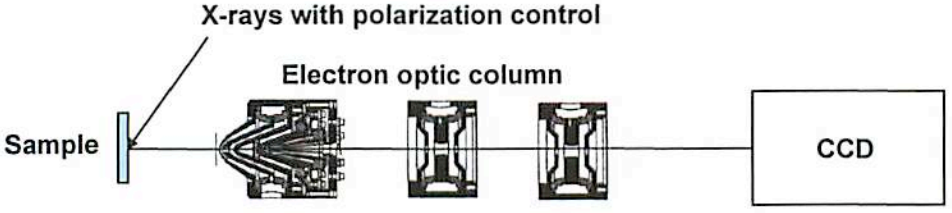


3D isosurface | Cross-section (bar = 200nm) | Res'n 20-30 nm

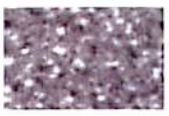
H. Chapman, M. Howells, A. Barty, S. Marchesini

PhotoEmission Electron Microscopy - PEEM

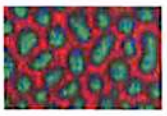
ALS PEEM allows measurements of composition, chemistry, and magnetic properties of surfaces and thin films at nanometer spatial and picosecond temporal resolution.



Examples



Sub 100 nm size magnetic pillars in a ferroelectric matrix
T. Zhao et al., Appl. Phys. Lett. 90, 123104 (2007)



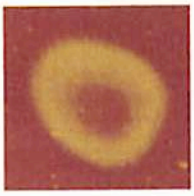
Protein adsorption on two segregated polymers
C. Morin et al., JES&RP 137-140, 785 (2004).

Magnetic phase transition in Fe
Y. Wu et al., Phys. Rev. Lett. 93, 117205 (2004)

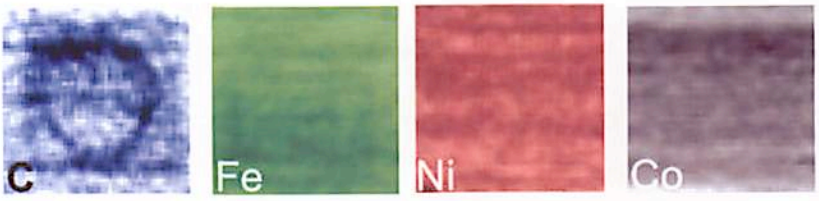
Vortex dynamics
S.B. Choe et al., ALS, Science 304, 420 (2004)

Magnetic XMCD STXM at 11.0.2 Reveals That ONLY Carbon is Magnetic

The area around the proton beam impact shows a magnetic signal in the AFM



AFM image -Field of view~4μm

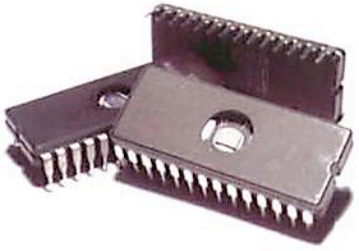


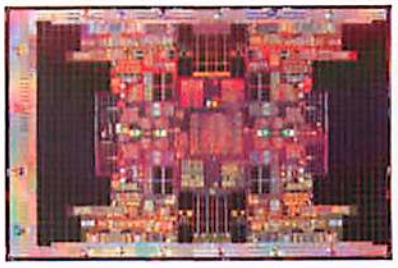
Element specific magnetic STXM images of the identical area

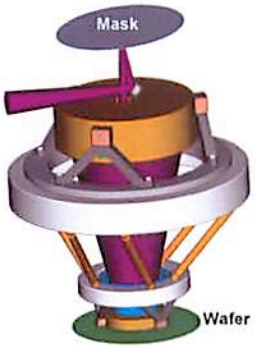
STXM images at BL11.0.2 reveals the "magnetic ring" is caused by long range magnetic order of carbon atoms only

H. Ohldag, T. Tyliszczak, R. Höhne, D. Spemann, et al, PRL 98, 187204 (2007)

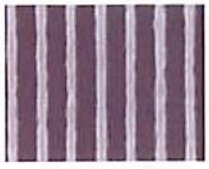
Extreme Ultraviolet Lithography for microchips of the future





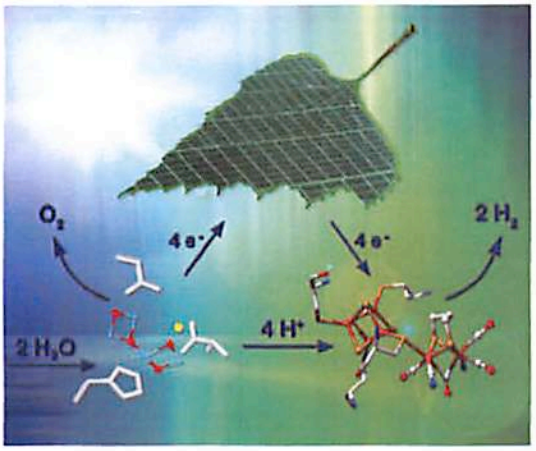


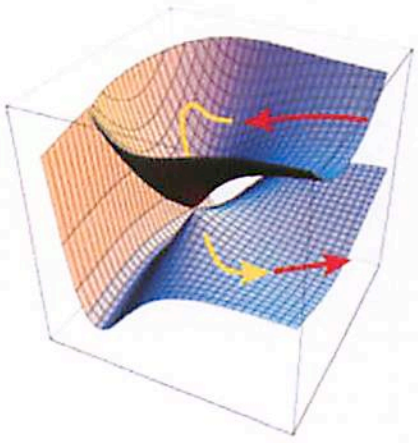
27 nm



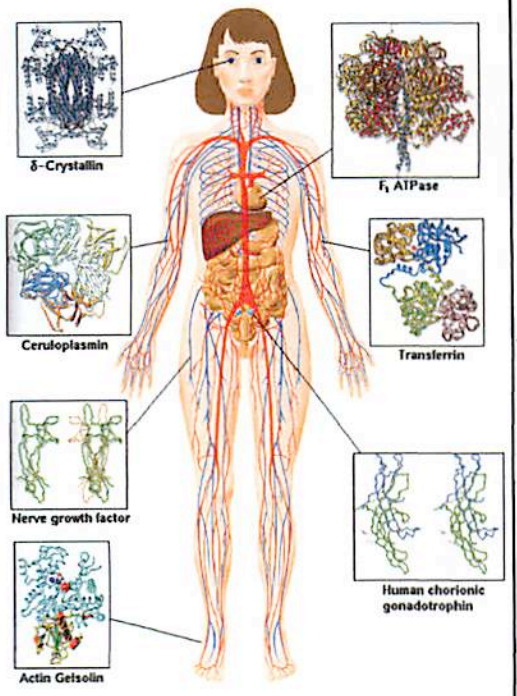
Sematech, Intel, AMD, IBM, Samsung and others

Understand ultrafast energy and information flow in molecular systems

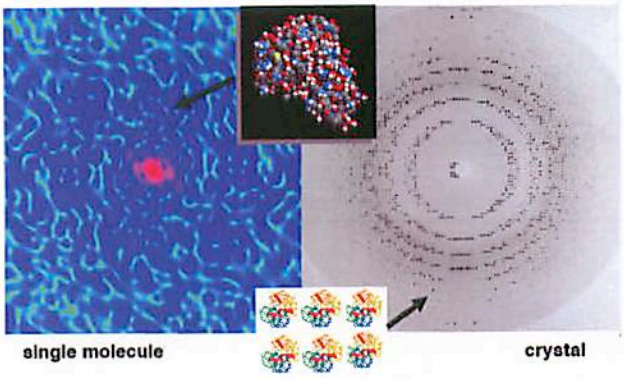


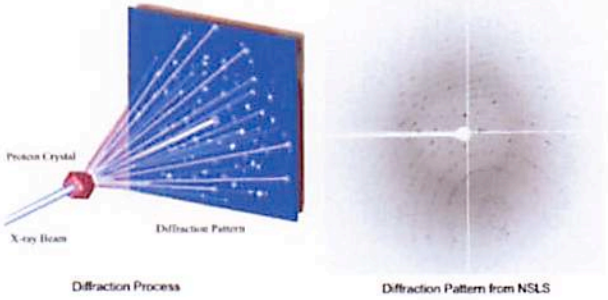


What is the atomic structure of biological proteins



Scattering by a single molecule and by a crystal





Macromolecular Crystallography: Eukaryotic Transcription

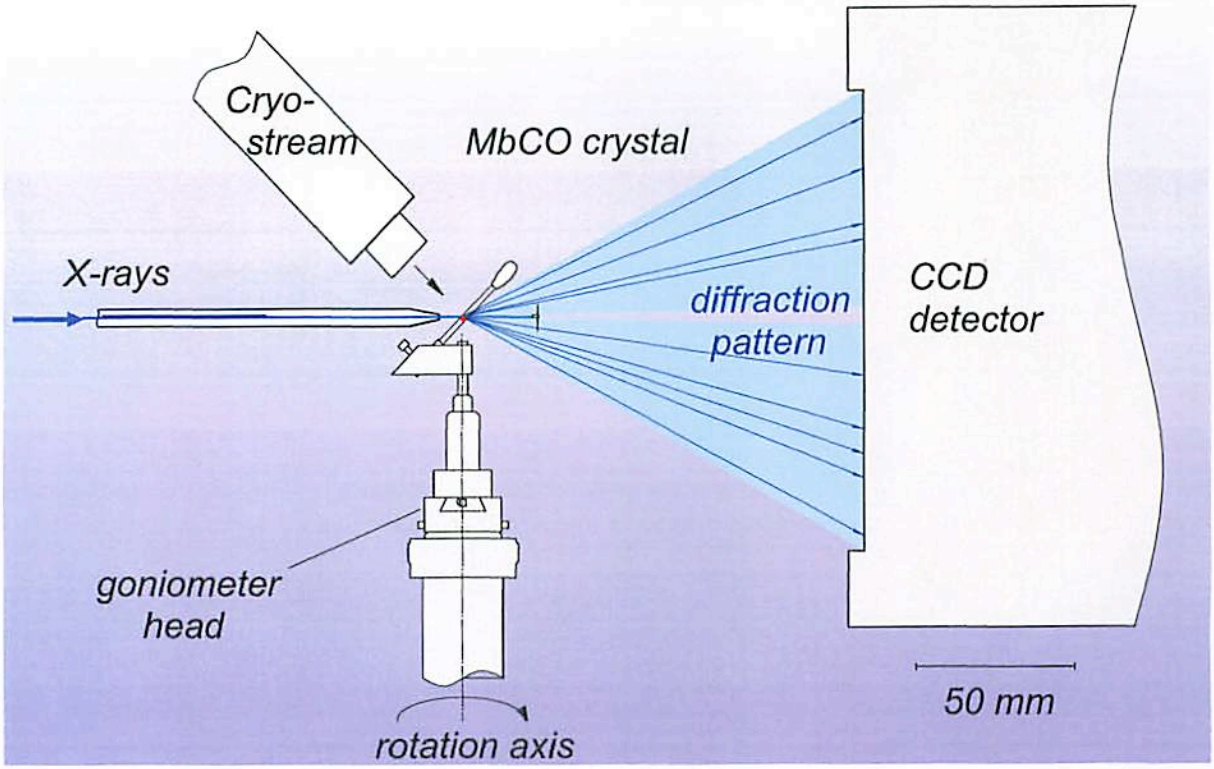
Transcription of the genetic code is essential to life. The genetic information is copied from DNA into messenger-RNA. This messenger carries the information out of the cell nucleus so that it can be translated into proteins. Crystallography has been vital in understanding the detailed mechanism of transcription.

2006 Nobel Laureate for Chemistry
Roger Kornberg

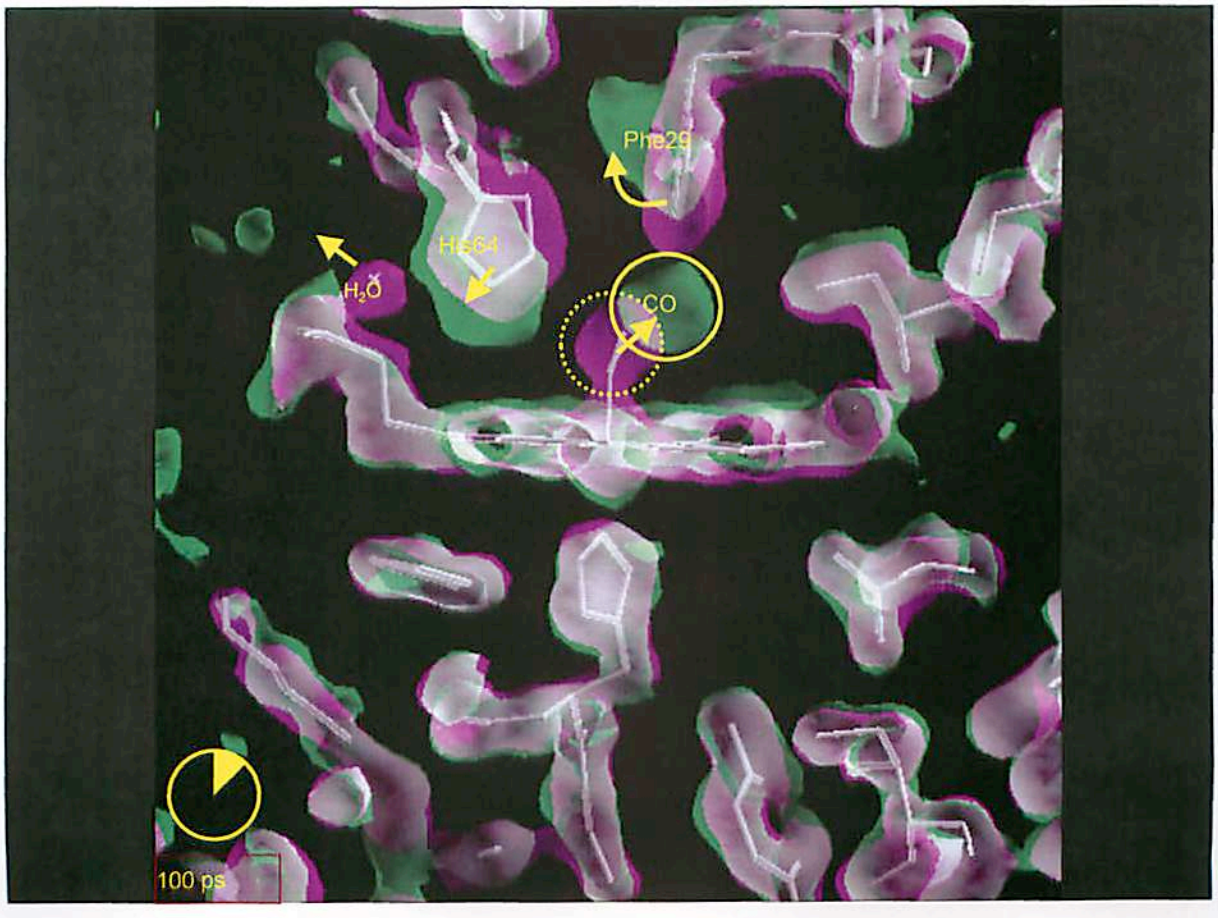
Kornberg used beamlines at the ALS as well as SSRL to determine the structure of RNA Polymerase II

Bushnell, D.A., K.D. Westover, R.E. Davis, and R.D. Kornberg, "Structural basis of transcription: an RNA polymerase II-TFIIB cocrystal at 4.5 Angstroms," Science 303, 983 (2004). (5.0.2, 8.2.1)

X-Ray crystalography (scattering of x-rays from crystals) reveals the atomic structure of complex proteins

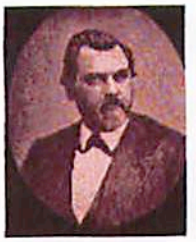



off
Science, 300, 194
(20 Jun 2003)

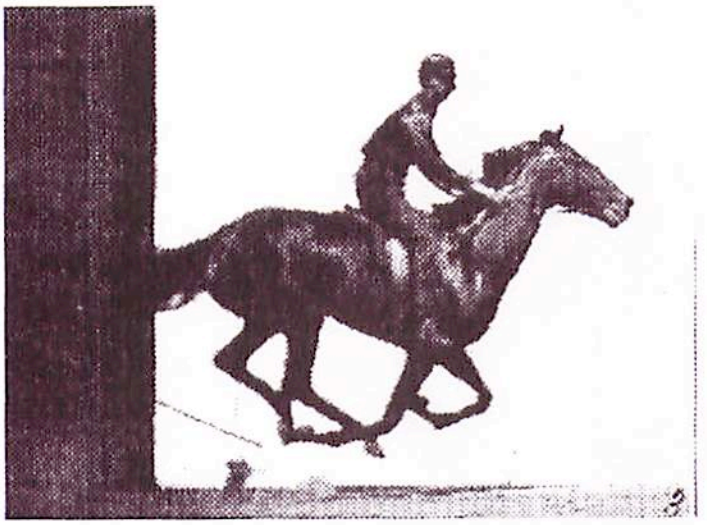

Phe29
His64
H_2O
CO
100 ps

E. Muybridge

Muybridge's "ultrafast" movie using spark photography Stanford University, 1878



L. Stanford

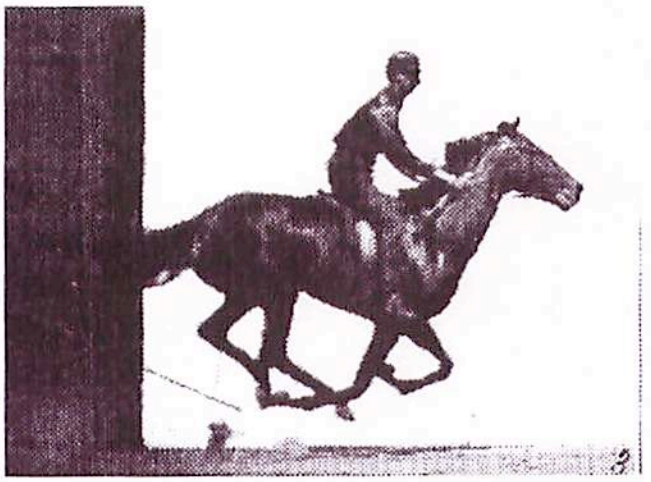


E. Muybridge, *Animals in Motion*, ed. by L. S. Brown (Dover Pub. Co., New York 1957).

E. Muybridge

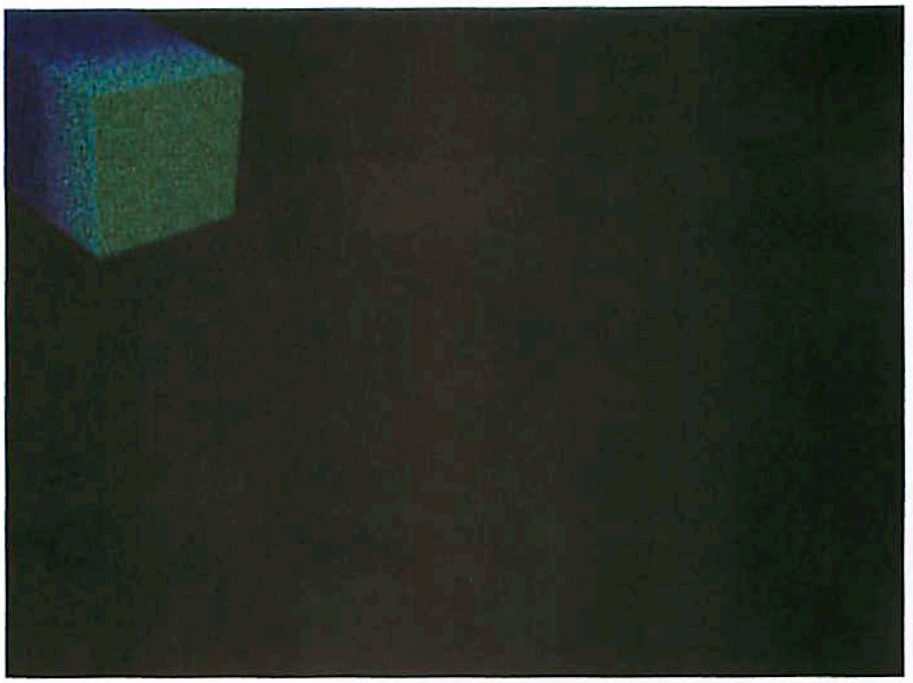
Muybridge's "ultrafast" movie using spark photography Stanford University, 1878

L. Stanford



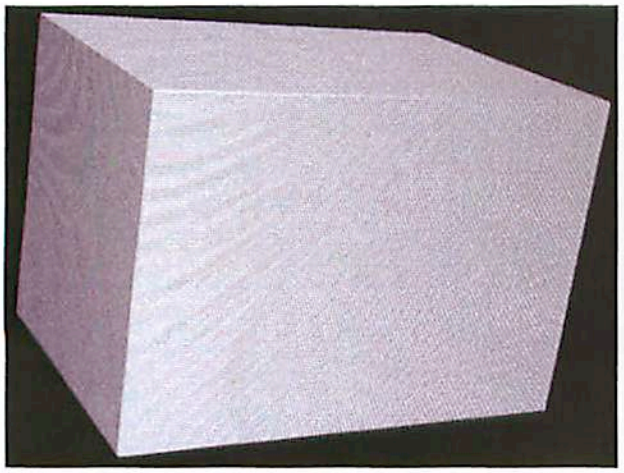
To see atomic motion, we need to shorten the wavelength by 10^4 and the time scale by 10^{13}

Ablation of a surface when quickly heated

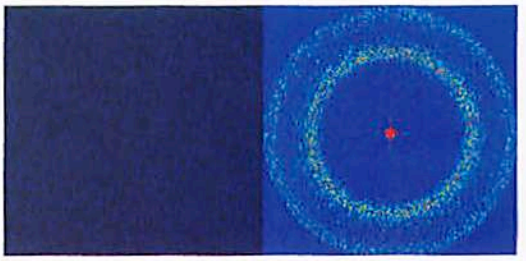


Intense shock pulse causes a phase transition

Grey = static BCC Blue = compressed BCC Red = HCP



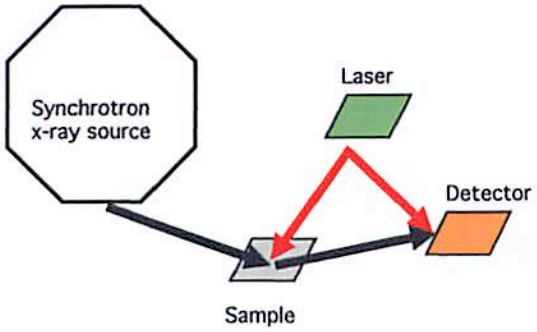
Atomic simulation of 8 million atoms by computer over a time period of 10 picoseconds

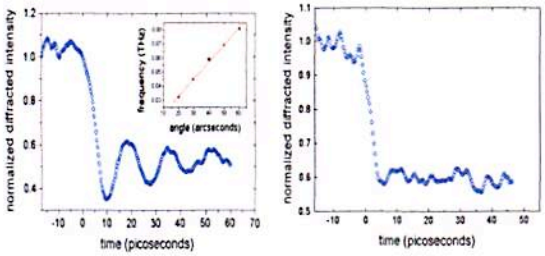


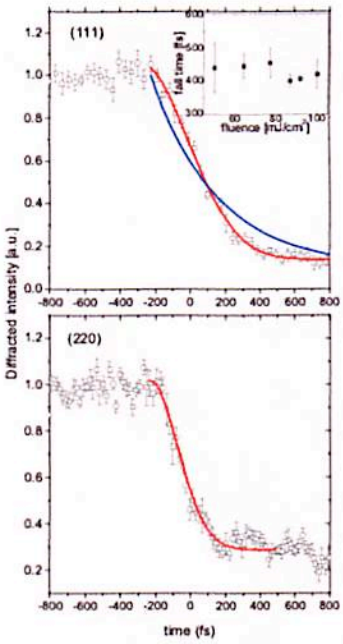
Simulation of measurement by ultrafast x-rays

This is theory, and we need experiments to test our ability to use computers to simulate the dynamic world !

Light shining on a metal can cause heating and melting.
Light shining on a material can also break molecular bonds, and "cold melt" it.
This can be observed by ultrafast x-rays.



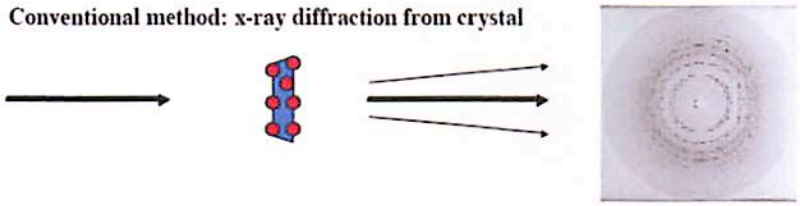




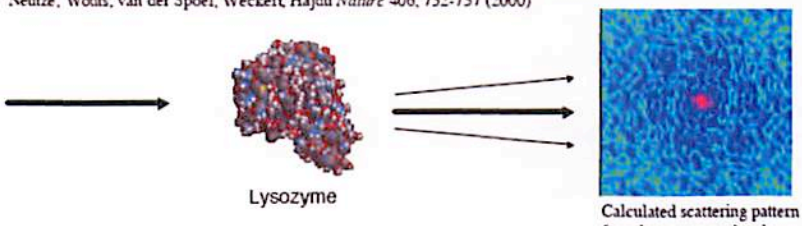
Lindenberg et al., Phys Rev. Lett. 84, 111 (2000)

Single molecule (nanocrystal, biomolecule) imaging has been proposed using short-pulse x-ray FELs

Conventional method: x-ray diffraction from crystal



Proposed method: diffuse x-ray scattering from single protein molecule
Neutze, Wouts, van der Spoel, Weckert, Hajdu *Nature* 406, 752-757 (2000)



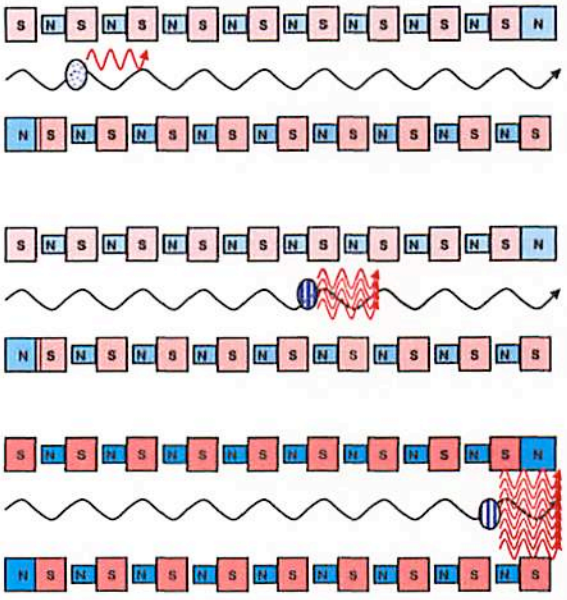
Lysozyme

Calculated scattering pattern from lysozyme molecule

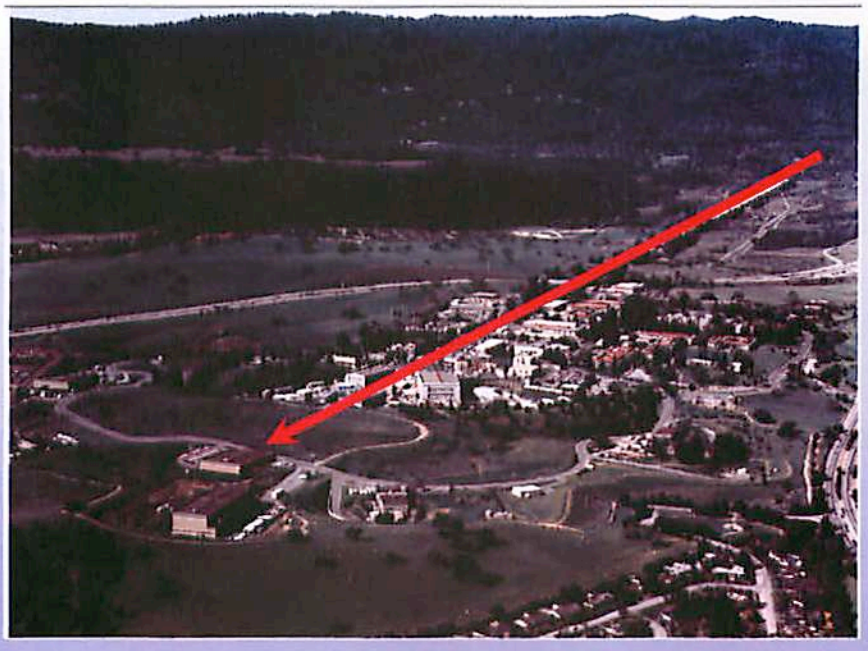
Implementation limited by radiation damage:

In **crystals** limit to damage tolerance is about **200 x-ray photons/Å²**
For **single protein molecules** need about **10^{10} x-ray photons/Å²** (for 2Å resolution)

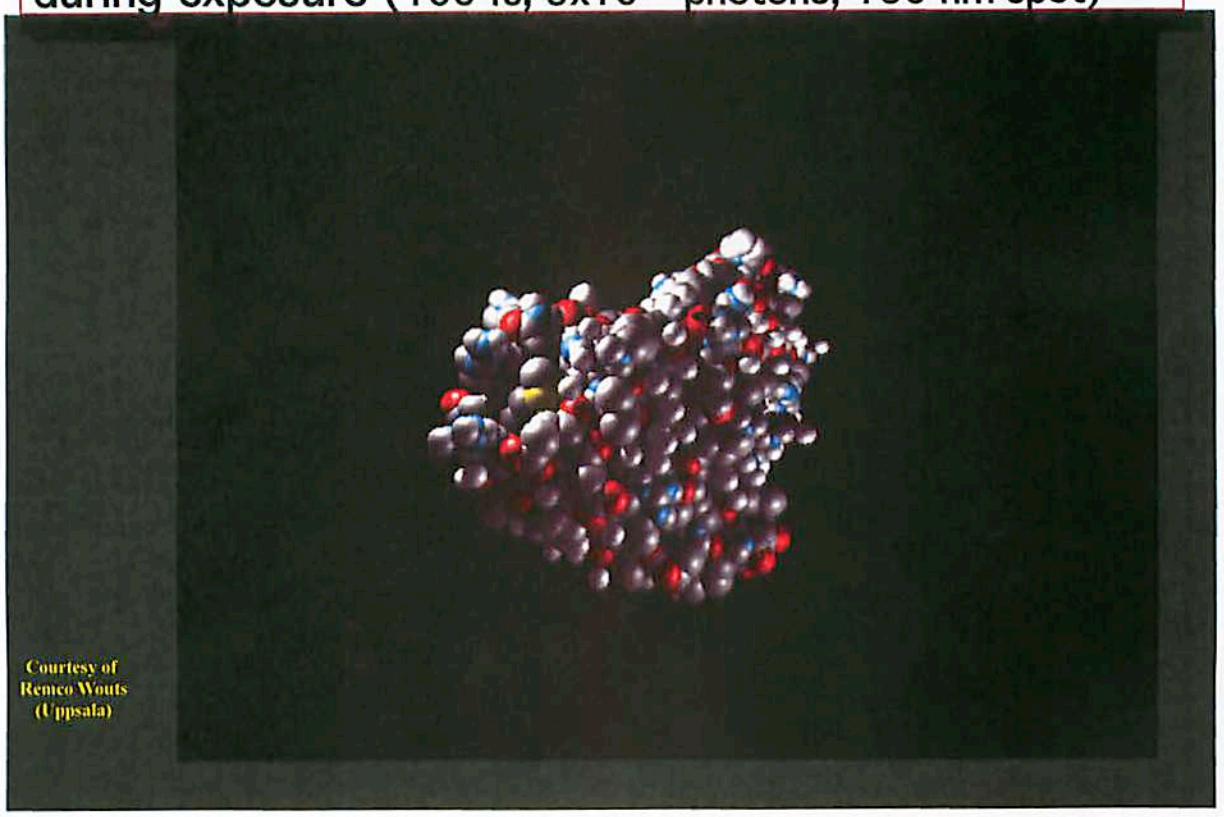
Long undulators and wigglers produce electron bunches that radiate intense and laser-like coherent x-rays



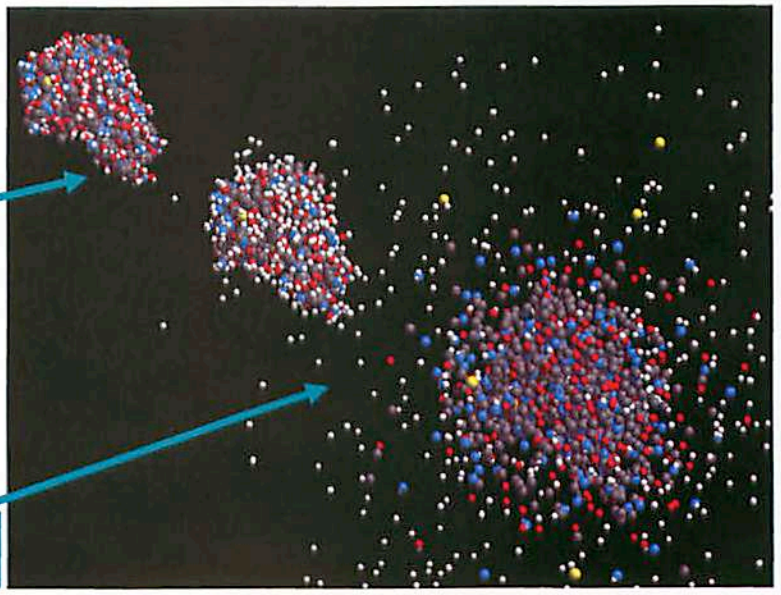
Stanford's SLAC LINAC will be a source of coherent x-ray pulses at the LCLS



Imaging single protein molecules causes movement during exposure (100 fs, 3×10^{10} photons, 100 nm spot)

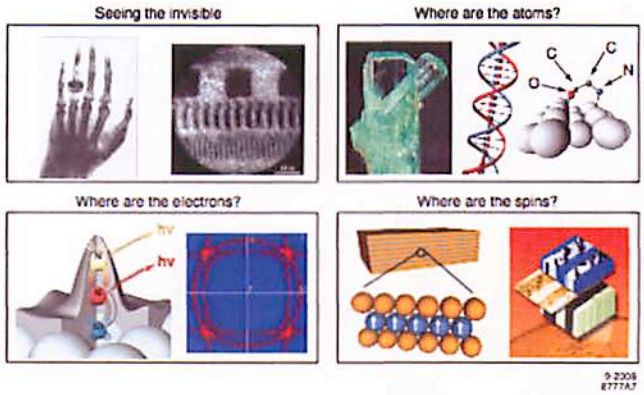


Computer simulations of the explosion of a protein molecule during imaging imply we need *very fast* x-ray pulses to take a picture of just one



from Neutze, Wouts, van der Spoel, Weckert, & Hajdu, Nature 406, 752 (2000)

Some conclusions



- X-Rays reveal where **atoms** are (the structure of materials), how atoms are **bonded** together in molecules and solids (the glue), and how they behave
- Fast processes are studied using pulses of x-rays; "fast" is used in **nature** to direct energy and information flow; we can study this to make better **technology**
  - ➢ beat the timescales for loss of energy into unwanted modes of the system
    - ▪ this is how vision & photosynthesis work
      - ✓ since we need efficient photovoltaics
  - ➢ allow dissipation of energy to minimize damage to a system
    - ▪ this is how DNA damage by light is prevented
      - ✓ since we need durable materials

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